National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 350b

Benzoic Acid (Acidimetric)

C_6H_5COOH

This Standard Reference Material (SRM) consists of highly purified benzoic acid (C_6H_5COOH). SRM 350b is intended for use in acidimetric standardization and is supplied in a unit of 30 g.

Certified Values and Uncertainties: The certified values, reported in Table 1 as a mass fraction ($w_{C_6H_5COOH}$) and amount-of-substance content of H^+ ion (ν_{H^+}), are based on coulometric assays of the dried material (see "Drying Instructions") including the effects of air buoyancy. The certified values are based on the results of determinations from 12 randomly selected bottles from the entire lot of SRM 350b. Each determination was obtained by coulometric acidimetric titration [1] to the inflection point (pH ca. 8.15).

Table 1. Certified Values for SRM 350b Benzoic Acid

$w_{C_6H_5COOH}$	99.9978 % ± 0.0044 %
ν_{H^+}	8.188 40 mol kg^{-1} ± 0.000 26 mol kg^{-1}

The uncertainties in Table 1 are expanded uncertainties, U, calculated as $U = ku_c$, where k is a coverage factor that governs the confidence level of U and u_c is the combined standard uncertainty calculated according to the ISO and NIST Guides [2]. The quantity u_c represents, at the level of one standard deviation, the potential combined effects of the uncertainty arising from instrumental sources, chemical interferences, and uncertainties in fundamental constants, and possible material inhomogeneity. The value of k is calculated from the effective degrees of freedom, ν_{eff}. The value $k = 1.96$, corresponding to $\nu_{eff} > 1000$, was used to obtain the cited value for U for $w_{C_6H_5COOH}$. The value $k = 1.97$, corresponding to $\nu_{eff} = 437$, was used to obtain the certified value of U for ν_{H^+}. The coverage factors were each chosen to obtain an approximate 95 % level of confidence.

Expiration of Certification: The certification of this SRM is valid until **01 July 2015**, within the measurement uncertainties specified, provided the SRM is handled and stored in accordance with the instructions given in this certificate. However, the certification is invalid if the SRM is damaged, contaminated, or modified.

Maintenance of Certification: NIST will monitor representative samples from this SRM lot over the period of its certification. If substantive changes occur that affect the certification before the expiration of certification, NIST will notify the purchaser. Registration (see attached sheet) will facilitate notification.

The coordination of the technical measurements leading to the certification of this SRM was performed by K.W. Pratt of the NIST Analytical Chemistry Division.

Stephen A. Wise, Chief
Analytical Chemistry Division

Gaithersburg, MD 20899
Certificate Issue Date: 16 December 2005

Robert L. Watters, Jr., Chief
Measurement Services Division

Statistical consultation was provided by W.F. Guthrie of the NIST Statistical Engineering Division.

The support aspects involved in the certification of this SRM were coordinated through the NIST Measurement Services Division.

Calculation of Certified Value: The certified value was obtained using the present value for the Faraday constant, 96 485.336 C_{90} mol^{-1} [3], currently recommended for coulometric determinations. Corrections for air buoyancy were made using the measured density of 1.3039 g cm^{-3} for SRM 350b. The molar mass of benzoic acid, 122.121 34 g mol^{-1} (calculated from [4]), was used to calculate $w_{C_6H_5COOH}$ from ν_{H^+}. The uncertainty [4] in this molar mass is included in the certified value of $w_{C_6H_5COOH}$. The certified value of $w_{C_6H_5COOH}$ is calculated from ν_{H^+} under the assumption that the replaceable H^+ derives from a substance of net formula $C_7H_6O_2$. No representation is made as to the mass fraction of any impurities present.

INSTRUCTIONS FOR USE

Drying Instructions: Dry at room temperature (22 °C to 23 °C) for 24 h in a desiccator over anhydrous $Mg(ClO_4)_2$. The change in mass on drying is less than 0.005 %, relative. Previous investigations [5] indicate that benzoic acid will not absorb moisture from the atmosphere if the relative humidity does not exceed 90 %.

Stability and Storage: This SRM should be stored in its original bottle at room temperature. It must be tightly re-capped after use and protected from moisture and light.

Homogeneity: Tests indicate that this SRM is homogeneous within the uncertainty limits for sample sizes greater than 300 mg. Samples less than 300 mg are not recommended in order to avoid possible inhomogeneity with smaller sample sizes.

Source of Material: The benzoic acid used for this SRM was obtained from a commercial source. The material was examined for compliance with the specification for reagent grade benzoic acid as specified by the American Chemical Society [6]. The material was found to meet or exceed these specifications in all respects.

REFERENCES

[1] Pratt, K.W.; *Automated, High-Precision Coulometry* II. *Strong and Weak Acids and Bases*; Anal. Chim. Acta, Vol. 289, pp. 135–142 (1994).

[2] ISO; *Guide to the Expression of Uncertainty in Measurement*; ISBN 92-67-10188-9, 1st ed., International Organization for Standardization: Geneva, Switzerland (1993); see also Taylor, B.N.; Kuyatt, C.E.; *Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results*; NIST Technical Note 1297, U.S. Government Printing Office: Washington, DC (1994); available at http://physics.nist.gov/Pubs/.

[3] Mohr, P.J.; Taylor, B.N.; *CODATA Recommended Values of the Fundamental Physical Constants*: 2002; Reviews of Modern Physics, Vol. 77(1), pp. 1–107 (2005); available at http://physics.nist.gov/cgi-bin/cuu/Value?f90|search_for=faraday

[4] Commission of Atomic Weights and Isotopic Abundances; *Atomic Weights of the Elements* 2001; Pure & Appl. Chem., Vol. 75(8), pp. 1107–1122 (2003).

[5] SRM 350a; *Benzoic Acid* (*Acidmetric*); National Bureau of Standards, U.S. Department of Commerce: Gaithersburg, MD (1981).

[6] *Reagent Chemicals*, 8th ed.; American Chemical Society: Washington, DC (1993).

Users of this SRM should ensure that the certificate in their possession is current. This can be accomplished by contacting the SRM Program at: telephone (301) 975-6776; fax (301) 926-4751; e-mail srminfo@nist.gov; or via the Internet http://www.nist.gov/srm.